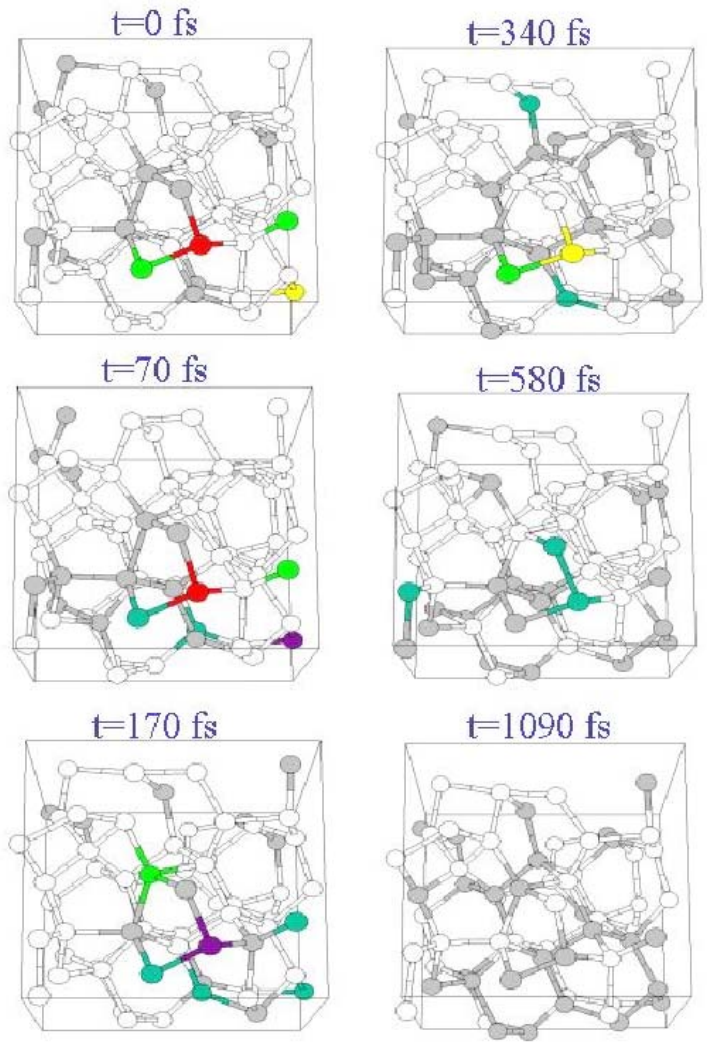
Electron hopping in amorphous silicon
Drabold, Ohio University, DMR 0081006

The motion of electrons in semiconductors is of key importance to technology and also raises questions of fundamental interest. Here, we compute the electron “hopping” in amorphous silicon (a material used in virtually all computer laptop displays and an important solar cell material). We employ accurate density functional methods to directly compute the thermally driven diffusion of the electrons from an (initially) spatially confined “localized” state into the rest of the model. We are studying the role of temperature, defects and impurities on this electronic motion. In the Figure, t is the time (in femtoseconds, 10^{-15} s), and the color coding is a measure of the charge. The ordering is red (>0.15 electron), purple, yellow, green, blue grey white (<1/64 electron). The figure is for a “band tail” state at room temperature. For this example, note that the electron rapidly diffuses across the model.



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Brief summary of outreach activities:

Educational:
1 undergraduates,
5 grad students,
2 post-docs.